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## Final Technical Report

Virginia Tech Graduate Student Support

HR00110710038

The massacre at the Virginia Polytechnic Institute and State University on April 16, 2007 is the greatest tragedy that U.S. higher education has faced. In an attempt to help its community cope with this heartbreaking event, the university administration decided to close Norris Hall, the site of many of the shootings. This closer caused about 60 researchers and students to be displaced and without laboratories for the summer to work on their research and dissertations. Through your support six of the displaced students came to the Advanced Technology Laboratory in The Johns Hopkins Whiting School of Engineering for approximately ten weeks so that their research was not further disrupted from the tragedy. The graduate students were each paired with a Whiting School faculty whose research interests and field of study were in line. The students worked on their current doctoral programs and the Johns Hopkins faculty helped to mentor the students. The student's ability to come to Johns Hopkins further enhanced their knowledge and fields of study and also allowed the students to not fall further behind due to the tragedy.

The following students and faculty were supported partially by DARPA funding:

- Aproova Shende, student
- Arun Nair, student
- Wen Jiang , student
- Kaushik Das, student
- Kalia Ramesh, Professor
- Kevin Hemker, Professor
- Takeru Igusa, Professor

Approva Shende's thesis work is on modeling pedestrian traffic in buildings during emergency evacuation using partial differential equations. Dr. Igusa worked with Shende by using smoothed particle hydrodynamics (SPH) as a computationally efficient algorithm to solve these equations.

This was a novel application because the particles in SPH, which are traditionally used to represent parcels of fluid, were used to represent pedestrians. Interactions between particles were modeled in terms of human behavior during emergency events and the boundary conditions were determined by the building geometry and evacuation routes.

Arun Nair and Kevin Hemker worked on atomistic simulations of materials in extreme environments. Specifically, he simulated the plastic deformation and movements of atoms under the tip of an indenter during nanoindentation in a way that helped us incorporate strain gradient plasticity in the model described below. His work related to an AFOSR supported MEANS-2 project that provided a pathway for describing TBC delamination in a way that incorporates: atomic-scale first-principles descriptions of interfacial bonding (as a function of chemistry); micro- and nano-scale measurements of plasticity (including strain gradient length scales); elastic behavior of the top and bond coats; and a continuum-level description of the stresses that develop during thermal cycling. This type of integrated length-scale modeling has never been accomplished

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before for a problem that incorporates atomistics with plasticity and fracture. It predicts trends in the toughness with stoichiometry, segregation and dopant, as a function of the yield strength of the bond coat adjacent to the interface and the characteristic plasticity length scale due to the geometrically-necessary dislocations that accumulate in the plastic zone.

Wen Jiang worked with Professor Kaliat Ramesh on molecular dynamics simulations of indentation problems, and on developing formulations for the indentation of a nonlinear elastic solid. Ms. Jiang was successful in work with Dr. Ramesh and has since graduated.

Kaushik Das and Matthew Lear worked together to develop a fully coupled fluid-structure-interaction simulation. Their technique was used to analyze the heating of a composite plate with a nano-tube surface coating exposed to a flow of hot gas. The results were then compared to available experiment data.

The following students and faculty also were supported by the National Science Foundation and the Applied Physics Laboratory by similar grants:

- Osama Marzouk, student
- Amanda Young, student
- Matthew Lear, scientist

The students felt that their time at Johns Hopkins was very helpful in the learning and healing process. They were very thankful for the opportunity to work on their research and to work with different mentors.